

Perturbation hydrogen-atom spectrum in deformed space with minimal length

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We study energy spectrum for hydrogen atom with deformed Heisenberg algebra leading to minimal length. We develop correct perturbation theory free of divergences. It gives a possibility to calculate analytically in the 3D case the corrections to s -levels of hydrogen atom caused by the minimal length. Comparing our result with experimental data from precision hydrogen spectroscopy an upper bound for the minimal length is obtained.

I. INTRODUCTION

Recently a lot of attention has been attracted to the quantum mechanical problems linked with generalized (modified) commutation relations. Such an interest was motivated by the works on quantum gravity and string theory which suggested the existence of a finite lower bound to the possible resolution of length (minimal length) [1, 2, 3]. Kempf et al. showed that minimal length can be obtained from the deformed Heisenberg algebra [4, 5, 6, 7, 8]. Note that for the first time the deformed algebra leading to quantized space-time was introduced by Snyder in the relativistic case [9]. In D-dimensional case the deformed algebra proposed by Kempf reads

$$\begin{aligned} [X_i, P_j] &= i\hbar(\delta_{ij}(1 + \beta P^2) + \beta' P_i P_j), \quad [P_i, P_j] = 0, \\ [X_i, X_j] &= i\hbar \frac{(2\beta - \beta') + (2\beta + \beta')\beta P^2}{1 + \beta P^2} (P_i X_j - P_j X_i), \end{aligned} \tag{1}$$

where β, β' are parameters of deformation. We suppose that these quantities are positive $\beta, \beta' \geq 0$. It can be seen that position operators do not commute so we have a noncommutative space. From the uncertainty relation it follows that minimal length is $\hbar\sqrt{\beta + \beta'}$.

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Note that in the special case $\beta' = 2\beta$ the position operators in linear approximation over deformation parameters commute, i.e. $[X_i, X_j] = 0$.

The hydrogen atom is one of the simplest quantum system allowing highly accurate theoretical prediction and is well studied experimentally offering the most precisely measured quantities [10]. Therefore, this simple atom has a crucial role for our understanding of key points of modern physics. Due to the singularity of the Coulomb potential at the origin this system is in particular sensitive to whether there is a fundamental minimal length. There are only a few papers on the investigation of hydrogen atom in quantum space with minimal length [11, 12, 13].

Brau [11] considered the special case of deformation $\beta' = 2\beta$ and in the linear approximation over the deformation parameters the energy spectrum of hydrogen atom was calculated. The general case of deformation $\beta' \neq 2\beta$ was studied in [12]. Using perturbation theory the authors calculated correction to the energy spectrum of hydrogen atom. But in order to calculate the corrections to s -levels for three dimensional space the authors were forced to use a numerical method and cut off procedure due to the appear once of the term $\sim 1/r^3$ in the Hamiltonian in linear approximation over β, β' . We would like to emphasize that without cut off procedure this term leads to divergence the correction to s -levels.

Note also paper [14] where the comparison between the "space curvature" effects and minimal length effects for the hydrogen spectrum was made. In [15] a one dimensional Coulomb problem was solved exactly.

In the present paper we propose the modified perturbation theory free of divergences which gives a possibility to calculate the corrections to all energy levels including s -levels. This paper is organized as follows. In the second section we obtain corrections to the spectrum of D -dimensional Coulomb problem using ordinal perturbation theory. In the third section we propose modified perturbation theory and calculate corrections to the energy of s -levels of hydrogen in three dimensional case. And finally fourth section contains the discussion.

II. PERTURBATION OF THE ENERGY SPECTRUM

In this section we consider ordinal perturbation theory similarly as in [12] but using another representation of the deformed algebra. This algebra is more convenient for the

development the modified perturbation theory.

We study the eigenvalue problem for hydrogen atom in D -dimensional case

$$\left(\frac{\mathbf{P}^2}{2m} - \frac{e^2}{R} \right) \Psi = E\Psi \quad (2)$$

where operators of position X_i and momentum P_i satisfy deformed commutation relation (1), $R = \sqrt{\sum_{i=1}^D X_i^2}$.

We use the following representation that satisfies the algebra (1) in the first order in β , β'

$$\begin{cases} X_i = x_i + \frac{2\beta - \beta'}{4} (x_i p^2 + p^2 x_i), \\ P_i = p_i + \frac{\beta'}{2} p_i p^2; \end{cases} \quad (3)$$

where $p^2 = \sum_{k=1}^D p_k^2$ and operators x_i, p_i obey canonical commutation relations $[x_i, p_j] = i\hbar\delta_{ij}$.

For the undeformed Heisenberg algebra the position representation may be taken: $x_i = x_i$, $p_i = i\hbar \frac{\partial}{\partial x_i}$.

We write Hamiltonian of equation (2) using representation (3) and taking into account only the first order terms in β, β'

$$H = \frac{p^2}{2m} + \frac{\beta' p^4}{2m} - \frac{e^2}{\sqrt{r^2 + \frac{2\beta - \beta'}{2} (r^2 p^2 + p^2 r^2 + \hbar^2 D)}} \quad (4)$$

where $r = \sqrt{\sum_{i=1}^D x_i^2}$ and D is the dimension of space.

Expanding the inverse distance R^{-1} in the series over parameters of deformation up to the first order β, β' we have

$$H = \frac{p^2}{2m} + \frac{\beta' p^4}{2m} - e^2 \left(\frac{1}{r} - \frac{2\beta - \beta'}{4} \left(\frac{1}{r} p^2 + p^2 \frac{1}{r} + \frac{\hbar^2 (D-1)}{r^3} \right) \right) \quad (5)$$

This Hamiltonian contains correction of first order over β, β' to undeformed hydrogen atom Hamiltonian.

Now we can calculate the corrections $\Delta E_{nl}^{(1)}$ to the spectrum using the eigenfunctions of undeformed hydrogen atom

$$\Delta E_{nl}^{(1)} = \frac{e^2 \hbar^2}{a^3 n^3} \left(\frac{(D-1)(2\beta - \beta')}{4\bar{l}(\bar{l}+1)(\bar{l}+\frac{1}{2})} + \frac{2\beta + \beta'}{\bar{l} + \frac{1}{2}} - \frac{\beta + \beta'}{\bar{n}} \right) \quad (6)$$

where a is the Bohr radius and $\bar{n} = n + \frac{D-3}{2}$, $\bar{l} = l + \frac{D-3}{2}$, n is the principal quantum number and l is the orbital quantum number.

Expression (6) is in agreement with the results calculated in the paper [12]. It is worth to mention that in the special case $D = 3$ and $l = 0$ expression (6) gives divergent contribution. It is caused by the term proportional to $1/r^3$ in Hamiltonian (5).

III. MODIFIED PERTURBATION THEORY. CORRECTIONS TO THE ENERGY OF s -LEVELS IN THREE DIMENSIONAL CASE

In this section we propose a modified perturbation theory which gives a possibility to overcome the problem of divergence of the corrections to s -levels in three dimensional case. The idea is to use a shifted expansion of inverse distance R^{-1} which does not contain divergent terms like $1/r^3$. So, we rewrite R as follows

$$R = \sqrt{r^2 + b^2 + \alpha(r^2 p^2 + p^2 r^2 + \hbar^2 D - \bar{b}^2)} \quad (7)$$

where $\alpha = (2\beta - \beta')/2$ and $b^2 = \alpha \bar{b}^2$. Next we consider the expansion over $\alpha(r^2 p^2 + p^2 r^2 + \hbar^2 D - \bar{b}^2)$ in the vicinity of a new point $r^2 + b^2$. We will choose the introduced parameter b from the condition that terms proportional to $1/r^3$ are absent in the series.

In the first order over α we can write

$$\sqrt{r^2 + b^2 + \alpha(r^2 p^2 + p^2 r^2 + \hbar^2 D - \bar{b}^2)} = \sqrt{r^2 + b^2} + \alpha \hat{C}. \quad (8)$$

Squaring left and right hand side of (8) and taking into account only the term of first order over α we obtain the following equation for operator \hat{C}

$$r^2 p^2 + p^2 r^2 + \hbar^2 D - \bar{b}^2 = r \hat{C} + \hat{C} r \quad (9)$$

In order to find \hat{C} we write the left side of (9) in the following form

$$r^2 p^2 + p^2 r^2 + \hbar^2 D - \bar{b}^2 = \frac{1}{2} \left(r \left(r p^2 + p^2 r + \frac{A}{r} \right) + \left(r p^2 + p^2 r + \frac{A}{r} \right) r \right), \quad (10)$$

where parameter $A = \hbar^2(D - 1) - \bar{b}^2$.

It is straightforward to show using (10) that

$$\hat{C} = \frac{1}{2} \left(r p^2 + p^2 r + \frac{A}{r} \right). \quad (11)$$

So we have the following expansion for the distance

$$R = \sqrt{r^2 + b^2} + \frac{\alpha}{2} \left(r p^2 + p^2 r + \frac{A}{r} \right). \quad (12)$$

It is easy to obtain the inverse distance R^{-1} using (12)

$$\begin{aligned} \frac{1}{R} &= \frac{1}{\sqrt{r^2 + b^2}} - \frac{\alpha}{2\sqrt{r^2 + b^2}} \left(r p^2 + p^2 r + \frac{A}{r} \right) \frac{1}{\sqrt{r^2 + b^2}} = \\ &= \frac{1}{\sqrt{r^2 + b^2}} - \frac{\alpha}{2} \left(\frac{1}{r} p^2 + p^2 \frac{1}{r} + \frac{A}{r^3} \right). \end{aligned} \quad (13)$$

The contributions $1/\sqrt{r^2 + b^2}$ in the second term of expansion (13) can be replaced with $1/r$ in the linear approximation over α . We demand that our expansion does not contain the terms proportional to $1/r^3$ so we conclude that $A = 0$, i.e.

$$b = \hbar\sqrt{\alpha(D - 1)}. \quad (14)$$

It should be noted that (13) takes place under condition $b^2 > 0$, i.e. $2\beta > \beta'$.

We rewrite Hamiltonian (4) applying expansion (13) as follows

$$H = \frac{p^2}{2m} + \frac{\beta' p^4}{2m} - e^2 \left(\frac{1}{\sqrt{r^2 + b^2}} - \frac{2\beta - \beta'}{4} \left(\frac{1}{r} p^2 + p^2 \frac{1}{r} \right) \right) = H_0 + V, \quad (15)$$

where H_0 is the Hamiltonian of undeformed hydrogen atom and perturbation caused by deformation is

$$V = \frac{\beta' p^4}{2m} - e^2 \left(\frac{1}{\sqrt{r^2 + b^2}} - \frac{1}{r} - \frac{2\beta - \beta'}{4} \left(\frac{1}{r} p^2 + p^2 \frac{1}{r} \right) \right). \quad (16)$$

Now we calculate the correction to the ground state energy of hydrogen atom caused by perturbation V . First let us consider correction which is connected with $1/\sqrt{r^2 + b^2} - 1/r$.

We have

$$\left\langle \Psi_{1s} \left| \frac{1}{\sqrt{r^2 + b^2}} \right| \Psi_{1s} \right\rangle = \frac{4}{a^3} (\pi ab \left(H_1 \left(\frac{2b}{a} \right) - Y_1 \left(\frac{2b}{a} \right) \right)) - \quad (17)$$

$$-\frac{\pi b^2}{2} \left(H_0 \left(\frac{2b}{a} \right) - Y_0 \left(\frac{2b}{a} \right) \right). \quad (19)$$

where H and Y are the Struve and the Bessel functions, respectively [18]. Then up to first order over α (or b^2)

$$\left\langle \Psi_{1s} \left| \frac{1}{\sqrt{r^2 + b^2}} - \frac{1}{r} \right| \Psi_{1s} \right\rangle = \frac{2b^2}{a^3} \left(\ln \frac{b}{a} + \gamma + \frac{1}{2} \right). \quad (20)$$

where $\gamma = 0.57721\dots$ is the Euler constant.

It is easy to calculate the contributions caused by the terms $\frac{1}{r} p^2 + p^2 \frac{1}{r}$ and p^4 . As a result the correction to the ground state energy reads

$$\Delta E_{1s}^{(1)} = \langle \Psi_{1s} | V | \Psi_{1s} \rangle = \frac{e^2 \hbar^2}{a^3} \left(3\beta + \beta' - (2\beta - \beta') \left(\ln \frac{\hbar^2 (2\beta - \beta')}{a^2} + 2\gamma + 1 \right) \right). \quad (21)$$

We also calculate the correction to the $2s$ -level

$$\Delta E_{2s}^{(1)} = \langle \Psi_{2s} | V | \Psi_{2s} \rangle = \frac{e^2 \hbar^2}{8a^3} \left(\frac{7\beta + 3\beta'}{2} - (2\beta - \beta') \left(\ln \frac{\hbar^2 (2\beta - \beta')}{4a^2} + 2\gamma + \frac{5}{2} \right) \right). \quad (22)$$

Note that in special case $2\beta = \beta'$ these results for energy levels reproduce the results of Brau [11].

Similarly as in [12] we introduce two parameters $\xi = \Delta x_{\min}/a$ and $\eta = \beta/(\beta + \beta')$ instead of β and β' , where the minimal length $\Delta x_{\min} = \hbar\sqrt{\beta + \beta'}$. We have already noticed that calculated corrections to the s -levels take place under conditions $2\beta - \beta' \geq 0$. The conditions for the parameters β, β' restrict the domain of variation for the parameter η . It is easy to verify that $\frac{1}{3} \leq \eta \leq 1$. We rewrite the correction for the $1s$ -level using the parameters η and ξ :

$$\Delta E_{1s}^{(1)} = \frac{e^2}{a} \xi^2 \left(2\eta + 1 - (3\eta - 1) \left(\ln \xi^2 (3\eta - 1) + 2\gamma + 1 \right) \right). \quad (23)$$

The correction to the $2s$ -level as the function of parameters ξ and η reads

$$\Delta E_{2s}^{(1)} = \frac{e^2}{8a} \xi^2 \left(\frac{1}{2} (4\eta + 3) - (3\eta - 1) \left(\ln \frac{\xi^2 (3\eta - 1)}{4} + 2\gamma + \frac{5}{2} \right) \right) \quad (24)$$

Energy of $1s$ -level and $2s$ -level as a function of parameter ξ for the fixed value η is presented in Fig.1 and Fig.2 respectively. Unit of energy in these figures is the absolute value of the ground state energy of undeformed hydrogen atom $E_0 = e^2/2a$.

Finally we can consider constraints on the minimal length. As it was noted [12], the best estimation of the minimal length can be obtained by including the contributions of the minimal length effects in the Lamb shift. The experimental Lamb shift for the $1s$ -level of hydrogen atom $L_{1s}^{\text{expt}} = 8172.837(22)$ MHz [16] is larger than the best theoretically obtained $L_{1s}^{\text{theor}} = 8172.731(40)$ MHz [17]. Assuming similarly as in [12] that the discrepancy between experimental and theoretical values $L_{1s}^{\text{expt}} - L_{1s}^{\text{theor}}$ is entirely attributed to the minimal length correction $\Delta E_{1s}^{(1)}$ we find upper bound for the minimal length.

So having relation (23) we can estimate the minimal length as a function of parameter η . The limit values of the minimal length are $\Delta x_{\min} = 1.64 \cdot 10^{-16}$ m for $\eta = 1/3$ and $\Delta x_{\min} = 2.86 \cdot 10^{-17}$ m for $\eta = 1$. Let us compare our results with the estimation obtained in [12] where it was shown that for $\eta = \frac{1}{3}$ the minimal length $(\Delta x_{\min})^{-1} = 1.75$ GeV or $\Delta x_{\min} = 1.13 \cdot 10^{-16}$ m and for $\eta = 1$ the minimal length $(\Delta x_{\min})^{-1} = 6.87$ GeV or equivalently $\Delta x_{\min} = 2.87 \cdot 10^{-17}$ m, where $1\text{m} = (\hbar c/e)(\text{eV})^{-1}$. The comparison of our results for the minimal length with results obtained in [12] for all values of parameter η is shown in Fig.3.

As one can see our result for energy levels as well as for estimation of the minimal length are in good agreement with the result obtained in the paper [12], especially for the $\eta = 1$.

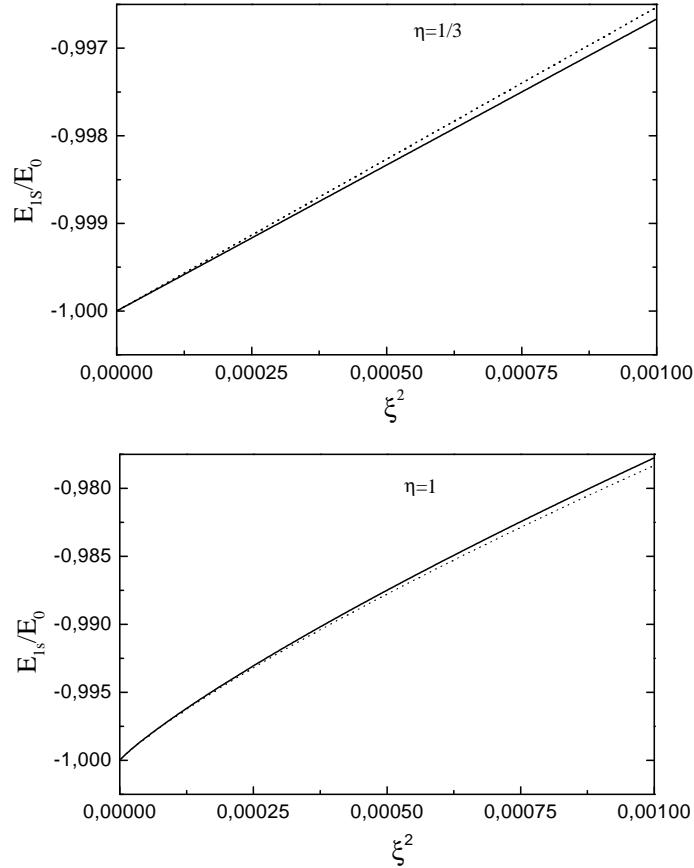


FIG. 1: Comparison of different results for the energy of 1s states with $\eta = 1/3$ (upper graph) and $\eta = 1$ (lower graph). Solid lines represent our results and dotted lines correspond to the results of Benczik [12].

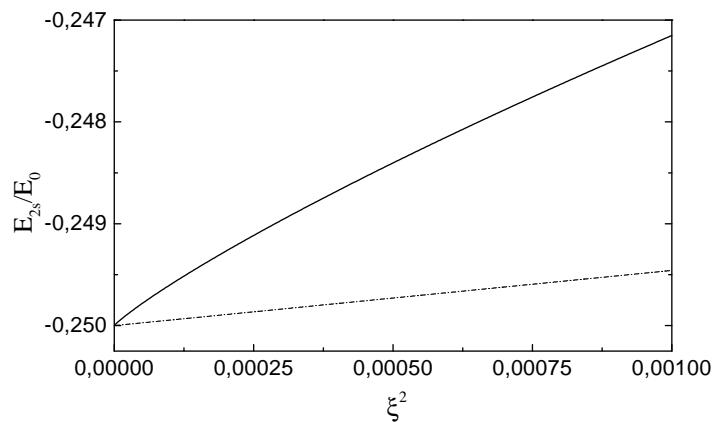


FIG. 2: Energy of 2s-level. Solid line shows the result when $\eta = 1$ and dash-dotted line corresponds the parameter $\eta = 1/3$.

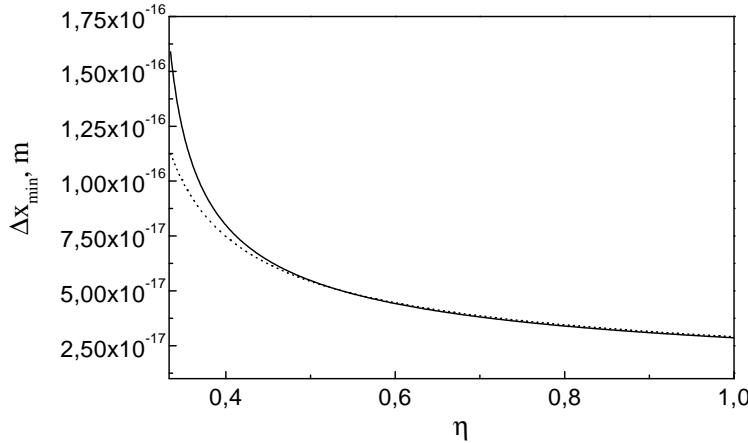


FIG. 3: Constraints on the minimal length as a function of dimensionless parameter η . Solid line represents the results obtained here and dotted line shows the results of [12].

The discrepancy between these two estimations are caused by the use different methods of computation. Namely, using modified perturbation theory we have analytical expressions for s -energy levels. The authors of [12] in order to calculate correction to s -levels in three dimensional case used cut off procedure and numerical calculation. More detailed comparison is made in Discussion.

IV. DISCUSSION

We study hydrogen atom in the space with deformed Heisenberg algebra leading to non-zero minimal length. The ordinary perturbation theory proposed in [12] leads to the term proportional to $1/r^3$ in perturbation operator. This term gives a divergent contribution to energy of s -levels in three dimensional case. Therefore, the authors of [12] were forced to use the cut off the expectation value integral $\langle 1/r^3 \rangle$ at some point. In order to find the free parameter appeared as a result of this procedure the author used the numerical calculation.

We construct a modified perturbation theory free of divergences where instead of b^2/r^3 we have $(1/r - 1/\sqrt{r^2 + b^2})$ with $b = \hbar\sqrt{(D-1)(2\beta - \beta')/2}$. It gives us a possibility to calculate analytically corrections to energy levels caused by deformation including s -levels in three dimensional case. Comparing our result with experimental data from precision hydrogen spectroscopy we find that the upper bound for the minimal length is of order 10^{-16} m, 10^{-17} m. Our results for energy levels as well as the result for estimation of the

minimal length are in a good agreement with the results obtained in the paper [12] with the help of numerical calculation and cut off procedure. Note also that for the case $\eta = 1/3$ ($2\beta = \beta'$) our results for energy levels reproduce the result of Brau [11], as it must be.

Finally, we would like to draw attention to the problem which is ignored in present paper as well as in the papers of other authors. Considering hydrogen atom in deformed space we suppose that Coulomb potential is the same as in non deformed space. In fact, in the deformed-space the Coulomb potential as a potential of a point charge might be corrected. This will lead to additional corrections to the energy spectrum of hydrogen atom. It is an interesting problem which worth separate investigations.

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